

coupledCahnHilliardAllenCahn formulation

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1 Outline

The weak formulations corresponding to the generic coupled phase field problem are derived, including the effects of interface energy anisotropy, but assuming isotropic mobility. Also, for now, the change in the normal direction due to mechanical deformation has not been included. The formulation will soon be extended to include variations of \mathbf{n} and anisotropic tensorial mobility.

2 Variational formulation

The total free energy of the system (neglecting boundary terms) is of the form,

$$\Pi(c, \eta) = \int_{\Omega_0} F(c, \eta) J dV \quad (1)$$

where dV represents a volume element in the reference configuration, $J = \det \mathbf{F}$ is the local volume change ratio and the free energy density is given by

$$F(c, \eta) = J \left(f(c, \eta) + \frac{1}{2} \nabla c \cdot \boldsymbol{\kappa}^c(\mathbf{n}) \nabla c + \frac{1}{2} \nabla \eta \cdot \boldsymbol{\kappa}^\eta(\mathbf{n}) \nabla \eta \right) \quad (2)$$

To account for anisotropic interfacial energy, $\boldsymbol{\kappa}^c$ and $\boldsymbol{\kappa}^\eta$ are assumed to be function of the interface orientation, given by the interface normal, \mathbf{n} . Subsequently, $\boldsymbol{\kappa}^c(\mathbf{n})$ and $\boldsymbol{\kappa}^\eta(\mathbf{n})$ can be reparametrized as $\boldsymbol{\kappa}^c(\theta, \phi)$ and $\boldsymbol{\kappa}^\eta(\theta, \phi)$, where (θ, ϕ) are the spherical coordinate angles. Also to begin with a simplified form of the orientation dependence is assumed:

$$\kappa_{ij}^c(\mathbf{n}) = \kappa^c(\mathbf{n}) \delta_{ij} \quad \kappa_{ij}^\eta(\mathbf{n}) = \kappa^\eta(\mathbf{n}) \delta_{ij} \quad (3)$$

Switching to the indicial notation and dropping explicit mentioning of the parametric dependence:

$$F = \left(f + \frac{1}{2} \kappa_{ij}^c c_{,i} c_{,j} + \frac{1}{2} \kappa_{ij}^\eta \eta_{,i} \eta_{,j} \right) \quad (4)$$

Now we proceed to derive the governing equations in the weak form.

3 Chemical dynamics (Cahn-Hilliard)

Considering variations of the form $c_\epsilon = c + \epsilon \omega$, the first variation of the free energy with respect to the concentration is given by:

$$\begin{aligned} \delta_c \Pi &= \left. \frac{d\Pi(c + \epsilon \omega, \eta)}{d\epsilon} \right|_{\epsilon=0} \\ &= \int_{\Omega_0} \frac{\partial f}{\partial c} \omega J dV \\ &+ \int_{\Omega_0} \kappa^c c_{,i} \omega_{,i} J dV \\ &+ \int_{\Omega_0} \left[\frac{\partial \kappa^c}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^c}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right] \omega_{,j} \frac{|\nabla c|}{2} J dV \end{aligned} \quad (5)$$

Integration by parts gives:

$$\begin{aligned}
\delta_c \Pi = & \int_{\Omega_0} \frac{\partial f}{\partial c} \omega J dV \\
& - \int_{\Omega_0} (\kappa^c c_{,i})_{,i} \omega J dV + \int_{\Gamma_0} \kappa^c c_{,i} n_i \omega J dS \\
& - \int_{\Omega_0} \left[\left(\frac{\partial \kappa^c}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^c}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla c|}{2} \right]_{,i} \omega J dV \\
& + \int_{\Gamma_0} \left[\left(\frac{\partial \kappa^c}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^c}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla c|}{2} \right] n_i \omega J dS
\end{aligned} \tag{6}$$

Collecting terms:

$$\begin{aligned}
\delta_c \Pi = & \int_{\Omega_0} \omega \left[\frac{\partial f}{\partial c} - (\kappa^c c_{,i})_{,i} - \left(\left(\frac{\partial \kappa^c}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^c}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla c|}{2} \right)_{,i} \right] J dV \\
& + \int_{\Gamma_0} \omega \left[\kappa^c c_{,i} + \left(\frac{\partial \kappa^c}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^c}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla c|}{2} \right] n_i J dS
\end{aligned} \tag{7}$$

From non-equilibrium thermodynamics we know that the volume integrand represents the chemical potential,

$$\mu = \frac{\partial f}{\partial c} - \mu^{grad} \tag{8}$$

$$\text{where } \mu^{grad} = (\chi_i)_{,i} \quad \text{and} \quad \chi_i = \kappa^c c_{,i} + \left(\frac{\partial \kappa^c}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^c}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla c|}{2}$$

if either $w|_{\Gamma_0} = 0$, that is no variation in the concentration field is allowed at the boundary, or if the surface integrand is assumed to vanish:

$$\begin{aligned}
& \left[\kappa^c c_{,i} + \left(\frac{\partial \kappa^c}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^c}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla c|}{2} \right] n_i = 0 \\
& \Rightarrow \chi_i n_i = 0
\end{aligned} \tag{9}$$

3.1 Governing equation

Now the statement of conservation of mass is given by:

$$\frac{\partial c}{\partial t} + (-L^c \mu_{,j})_{,j} = 0 \tag{10}$$

Again to begin with, the mobility is assumed to be a constant scalar. Since the finite element implementation is based on the weak formulation, we construct the weak form of Equation (10):

$$\begin{aligned}
& \int_{\Omega_0} \omega \left[\frac{\partial c}{\partial t} + (-L^c \mu_{,j})_{,j} \right] J dV = 0 \\
\Rightarrow & \int_{\Omega_0} \omega \left[\frac{\partial c}{\partial t} + \left(-L^c \left(\frac{\partial f}{\partial c} - \mu^{grad} \right)_{,j} \right)_{,j} \right] J dV = 0
\end{aligned} \tag{11}$$

Integration by parts twice gives the following formulation for chemical dynamics:

$$\begin{aligned} \Rightarrow & \int_{\Omega_0} \omega \frac{\partial c}{\partial t} + \int_{\Omega_0} \omega_{,j} L^c \left(\frac{\partial f}{\partial c} \right)_{,j} JdV - \int_{\Gamma_0} \omega L^c \left(\frac{\partial f}{\partial c} \right)_{,j} n_j JdS \\ & - \int_{\Omega_0} \omega_{,j} L^c \mu_{,j}^{grad} JdV + \int_{\Gamma_0} \omega L^c \mu_{,j}^{grad} n_j JdS = 0 \end{aligned} \quad (12)$$

$$\begin{aligned} \Rightarrow & \int_{\Omega_0} \omega \frac{\partial c}{\partial t} + \int_{\Omega_0} \omega_{,j} L^c \left(\frac{\partial f}{\partial c} \right)_{,j} JdV - \int_{\Gamma_0} \omega L^c \left[\left(\frac{\partial f}{\partial c} \right)_{,j} - \mu_{,j}^{grad} \right] n_j JdS \\ & + \int_{\Omega_0} \omega_{,jj} L^c \mu^{grad} JdV - \int_{\Gamma_0} \omega_{,j} n_j L^c \mu^{grad} JdS = 0 \end{aligned} \quad (13)$$

One can note that this equation involves only upto second order gradients of the concentration, with the second order gradients being part of the μ^{grad} term. However this is not the full weak form, because if we try to obtain the strong form starting with Equation (13) we simply revert to Equation (11) which only has the PDE without information about the boundary conditions. So with the knowledge of the boundary condition terms from Equation (13), we obtain the consistent weak formulation by adding two additional surface integral terms to Equation (13),

$$\begin{aligned} \Rightarrow & \int_{\Omega_0} \omega \frac{\partial c}{\partial t} + \int_{\Omega_0} \omega_{,j} L^c \left(\frac{\partial f}{\partial c} \right)_{,j} JdV - \int_{\Gamma_0} \omega L^c \left[\left(\frac{\partial f}{\partial c} \right)_{,j} - \mu_{,j}^{grad} \right] n_j JdS \\ & + \int_{\Omega_0} \omega_{,jj} L^c \mu^{grad} JdV - \int_{\Gamma_0} \omega_{,j} n_j L^c \mu^{grad} JdS \\ & + \int_{\Gamma_0} \omega \left(L^c \left[\left(\frac{\partial f}{\partial c} \right)_{,j} - \mu_{,j}^{grad} \right] n_j - \mathcal{J} \right) JdS + \int_{\Gamma_0} \omega_{,j} n_j L^c \left(\mu^{grad} - \mathcal{M} \right) JdS = 0 \end{aligned} \quad (14)$$

where \mathcal{J} and \mathcal{M} are the flux term and a chemical potential like term, respectively. The resulting consistent weak formulation is given by:

$$\Rightarrow \int_{\Omega_0} \omega \frac{\partial c}{\partial t} + \int_{\Omega_0} \omega_{,j} L^c \left(\frac{\partial f}{\partial c} \right)_{,j} JdV + \int_{\Omega_0} \omega_{,jj} L^c \mu^{grad} JdV - \int_{\Gamma_0} \omega \mathcal{J} JdS - \int_{\Gamma_0} \omega_{,j} n_j L^c \mathcal{M} JdS = 0 \quad (15)$$

Remark: The last term in the above equation vanishes for the special case of isotropic interfacial energy, as than Equation (9) reduces to a higher order dirichlet condition $c_j n_j = 0$, which implies $w_j n_j = 0$.

3.2 Mixed formulation

Instead of the weak form given by Equation (15), we develop the weak forms of Equations (8, 11). In addition to the concentration, we treat the chemical potential also as a primal field and the resulting two-field formulation is given below:

$$\int_{\Omega_0} \omega \left(\mu - \frac{\partial f}{\partial c} + \mu^{grad} \right) JdV = 0 \quad (16)$$

$$\int_{\Omega_0} \omega \left(\frac{\partial c}{\partial t} + (-L^c \mu_{,j})_{,j} \right) JdV = 0 \quad (17)$$

Using $\mu^{grad} = (\chi_i)_{,i}$ and integration by parts results in:

$$\int_{\Omega_0} \omega \mu JdV - \int_{\Omega_0} \omega \frac{\partial f}{\partial c} JdV - \int_{\Omega_0} \omega_{,i} \chi_i JdV + \int_{\Gamma_0} \omega \chi_i n_i JdS = 0 \quad (18)$$

$$\int_{\Omega_0} \omega \frac{\partial c}{\partial t} JdV + \int_{\Omega_0} \omega_{,j} L^c \mu_{,j} JdV - \int_{\Gamma_0} \omega L^c \mu_{,j} n_j JdS = 0 \quad (19)$$

Thus Equation (15) involving second order gradients of the primal field has been reduced to two equations involving first order gradients of the primal fields. However, in general mixed formulations increase the degrees of freedom of the system, may throw up non-physical boundary conditions, and result in decreased numerical stability (LBB conditions).

4 Structural order parameter dynamics (Allen-Cahn)

Considering variations of the form $\eta_\epsilon = \eta + \epsilon\omega$, the first variation of the free energy with respect to the order parameter is given by:

$$\begin{aligned}
\delta_\eta \Pi &= \left. \frac{d\Pi(c, \eta + \epsilon\omega)}{d\epsilon} \right|_{\epsilon=0} \\
&= \int_{\Omega_0} \frac{\partial f}{\partial \eta} \omega J dV \\
&\quad + \int_{\Omega_0} \kappa^\eta \eta_{,i} \omega_{,i} J dV \\
&\quad + \int_{\Omega_0} \left[\frac{\partial \kappa^\eta}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^\eta}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right] \omega_{,j} \frac{|\nabla \eta|}{2} J dV
\end{aligned} \tag{20}$$

Integration by parts gives:

$$\begin{aligned}
\delta_\eta \Pi &= \int_{\Omega_0} \frac{\partial f}{\partial \eta} \omega J dV \\
&\quad - \int_{\Omega_0} (\kappa^\eta \eta_{,i})_{,i} \omega J dV + \int_{\Gamma_0} \kappa^\eta \eta_{,i} n_i \omega J dS \\
&\quad - \int_{\Omega_0} \left[\left(\frac{\partial \kappa^\eta}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^\eta}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla \eta|}{2} \right]_{,i} \omega J dV \\
&\quad + \int_{\Gamma_0} \left[\left(\frac{\partial \kappa^\eta}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^\eta}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla \eta|}{2} \right] n_i \omega J dS
\end{aligned} \tag{21}$$

Collecting terms:

$$\begin{aligned}
\delta_\eta \Pi &= \int_{\Omega_0} \omega \left[\frac{\partial f}{\partial \eta} - (\kappa^\eta \eta_{,i})_{,i} - \left(\left(\frac{\partial \kappa^\eta}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^\eta}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla \eta|}{2} \right)_{,i} \right] J dV \\
&\quad + \int_{\Gamma_0} \omega \left[\kappa^\eta \eta_{,i} + \left(\frac{\partial \kappa^\eta}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^\eta}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla \eta|}{2} \right] n_i J dS
\end{aligned} \tag{22}$$

Again if we assume that the surface integrand vanishes,

$$\left[\kappa^\eta \eta_{,i} + \left(\frac{\partial \kappa^\eta}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^\eta}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla \eta|}{2} \right] n_i = 0 \tag{23}$$

than the governing equation for the structural order parameter dynamics is derived below. For ease of derivation we introduce the following notation:

$$\zeta = \frac{\partial f}{\partial \eta} - \zeta^{grad} \tag{24}$$

$$\text{where } \zeta^{grad} = (\chi_i^\eta)_{,i} \quad \text{and} \quad \chi_i^\eta = \kappa^\eta \eta_{,i} + \left(\frac{\partial \kappa^\eta}{\partial \theta} \frac{\partial \theta}{\partial n_i} + \frac{\partial \kappa^\eta}{\partial \phi} \frac{\partial \phi}{\partial n_i} \right) \frac{|\nabla \eta|}{2}$$

4.1 Governing equation

The governing equation for the non-conserved structural order parameter is given by:

$$\frac{\partial \eta}{\partial t} + L^\eta \zeta = 0 \tag{25}$$

Again the mobility is assumed to be a constant scalar. Now the corresponding weak form is given by:

$$\begin{aligned} \int_{\Omega_0} \omega \left[\frac{\partial \eta}{\partial t} + L^\eta \zeta \right] JdV &= 0 \\ \Rightarrow \int_{\Omega_0} \omega \left[\frac{\partial \eta}{\partial t} + L^\eta \left(\frac{\partial f}{\partial \eta} - (\chi_i^\eta)_{,i} \right) \right] JdV &= 0 \end{aligned} \quad (26)$$

Integration by parts gives the following formulation for order parameter dynamics:

$$\Rightarrow \int_{\Omega_0} \omega \frac{\partial \eta}{\partial t} JdV + \int_{\Omega_0} \omega L^\eta \frac{\partial f}{\partial \eta} JdV + \int_{\Omega_0} \omega_{,i} L^\eta \chi_i^\eta JdV - \int_{\Gamma_0} \omega L^\eta \chi_i^\eta n_i JdS = 0 \quad (27)$$

However this is not the full weak form, because if we try to obtain the strong form starting with Equation (27) we simply revert to Equation (26) which only has the PDE without information about the boundary conditions. So with the knowledge of the boundary condition terms from Equation (27), we obtain the consistent weak formulation by adding an additional surface integral term to Equation (27),

$$\begin{aligned} \Rightarrow \int_{\Omega_0} \omega \frac{\partial \eta}{\partial t} JdV + \int_{\Omega_0} \omega L^\eta \frac{\partial f}{\partial \eta} JdV + \int_{\Omega_0} \omega_{,i} L^\eta \chi_i^\eta JdV - \int_{\Gamma_0} \omega L^\eta \chi_i^\eta n_i JdS \\ + \int_{\Gamma_0} \omega L^\eta (\chi_i^\eta n_i - \mathcal{J}^\eta) JdS = 0 \end{aligned} \quad (28)$$

where \mathcal{J}^η is the boundary flux term. The resulting consistent weak formulation is given by:

$$\Rightarrow \int_{\Omega_0} \omega \frac{\partial \eta}{\partial t} JdV + \int_{\Omega_0} \omega L^\eta \frac{\partial f}{\partial \eta} JdV + \int_{\Omega_0} \omega_{,i} L^\eta \chi_i^\eta JdV - \int_{\Gamma_0} \omega L^\eta \mathcal{J}^\eta JdS = 0 \quad (29)$$